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Stability results for approximation by positive definite functions on SO(3)

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Abstract

We consider interpolation methods defined by positive definite functions on a locally compact group G. Estimates for the smallest and largest eigenvalue of the interpolation matrix in terms of the localization of the positive definite function on G are presented, and we provide a method to get positive definite functions explicitly on compact semisimple Lie groups. Finally, we apply our results to construct well-localized positive definite basis functions having nice stability properties on the rotation group $\mathrm{SO}(3)$.

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1. Introduction

Approximating a function f by linear combinations of a given single basis function ψ is a widely used method. The case where the underlying set is $\mathbb{R}^d$ and the basis function is radially symmetric (radial basis function) has been studied in great detail during the last decade (see [20] and references therein). Usually the setting is as follows. Given a data set $\mathcal{S} = \{(\mathbf{x}_1, f_1), \ldots, (\mathbf{x}_M, f_M)\} \subset \mathbb{R}^d \times \mathbb{R}$ and a basis function $\psi : \mathbb{R}_+ \to \mathbb{R}$, we suppose the f_i's to be point evaluations of an unknown function f. Now one tries to recover f by a linear combination of translates of the radial

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function $\psi(|\cdot|)$, i.e. we have an ansatz of the following type:

$$s(\mathbf{x}) = \sum_{k=1}^{M} a_k \psi(|\mathbf{x} - \mathbf{x}_k|), \quad \mathbf{x} \in \mathbb{R}^d.$$

Assuming that s interpolates the data leads to a system of linear equations for the coefficients a_k, i.e.

$$\mathbf{A}_\psi \mathbf{a} = \mathbf{f},$$

where $\mathbf{A}_\psi = (\psi(|\mathbf{x}_i - \mathbf{x}_k|))_{i,k=1}^M$, $\mathbf{a} = (a_k)_{k=1}^M$ and $\mathbf{f} = (f_k)_{k=1}^M$. It turns out that positive definite radial functions ψ are a good choice as basis functions in this setting. A radial function $\psi : \mathbb{R}_+ \to \mathbb{R}$ is called *positive definite* if

$$\sum_{j=1}^{M} \sum_{k=1}^{M} c_j \overline{c_k} \psi(|\mathbf{x}_j - \mathbf{x}_k|) \geqslant 0 \tag{1}$$

for all finite sets of points $\mathbf{x}_1, \ldots, \mathbf{x}_M \in \mathbb{R}^d$ and arbitrary coefficients $c_1, \ldots, c_M \in \mathbb{C}$. If the inequality (1) is strict for pairwise distinct $\mathbf{x}_j$'s, ψ is called a *strictly positive definite* radial basis function. Although for a strictly positive definite function (1) guarantees the invertibility of $\mathbf{A}_\psi$, the condition number of the interpolation matrix can be almost arbitrarily bad. The condition number depends strongly on how the sampling points are distributed. This means the process of determining the vector $\mathbf{a}$ can be unstable. A careful analysis shows how the condition number of the matrix depends on the one hand, on the so-called separation distance of the points and, on the other hand, on the specific properties of the basis function ψ. Besides $\mathbb{R}^d$, there also exist stability results for analogous interpolation methods in certain other settings. In [15], Narcowich et al. showed how the condition number can be controlled using suitable basis functions on the sphere. Kunis and Potts [11] studied the stability of scattered data interpolation on the torus $\mathbb{T}^d$ by multivariate trigonometric polynomials.

In various applications we are confronted with the situation where the underlying set is a compact or locally compact group G, i.e. $\mathcal{S}$ is now a subset of $G \times \mathbb{C}$. These types of problems arise, for example, in biochemistry and crystallography. In biochemistry, the protein docking problem is of great interest. In order to compute the docking correlation profiles efficiently, non-equispaced fast Fourier methods and basis function methods have to be developed, see [3] for details. In crystallography, basis function methods are utilized in order to interpolate the so-called pole figure intensities which are related to the orientations of a crystal in three-dimensional space. This means the orientations are related to certain points in $\mathsf{SO}(3)$. For more details on this problem we refer to [1,17]. Besides these applications, the problem of scattered data approximation on $\mathsf{SO}(3)$ arises in robotics. The so-called motion planning is one of the main issues in this field. The planning algorithms use normally irregular grids on $\mathsf{SO}(3)$, see [21].

The rotation group $\mathsf{SO}(3)$ is not the only group of relevance in science and engineering. In many situations special matrix groups are involved. The monograph [4] provides a great collection of problems where different matrix groups play an important role.

In the case where a locally compact group different from $\mathbb{R}^d$ is involved, the theory is by no means as well developed as in the classical setting. A main problem is to come up with suitable positive definite functions. As long as the group can be embedded in the Euclidean space $\mathbb{R}^d$, as in the case of matrix groups, one might try to restrict positive definite functions on $\mathbb{R}^d$ to the manifold defined by the group. Some work in this direction has been done by Levesley and Ragozin [12] and Narcowich [14]. In [2], the authors studied properties of positive definite functions on the sphere which are constructed in this way. The drawback of this approach is that we ignore the algebraic structure completely. It is better to work directly on the group. In this paper we are using algebraic concepts from the theory of Lie groups in order to construct a family of positive definite functions. For this purpose, we utilize the one-to-one relation between positive definite functions and unitary representations. This construction which is given for a general semisimple compact Lie group at first is later specialized to the rotation group $\mathsf{SO}(3)$. In this way we obtain a collection of positive definite functions Φ_n, where the parameter n controls the localization of the function. Given a data set on $\mathsf{SO}(3)$ with a certain separation distance we will show how to choose a suitable function out of the family that ensures that the interpolation process is stable. This means we derive estimates for the largest and the smallest eigenvalue of the interpolation matrix.

The paper is organized as follows. After collecting the basics on positive definite functions in the next section, we state our general stability result in Section 3. Next, we show in Section 4 how to get a family of positive definite functions in the case of a compact semisimple Lie group. Section 5 is devoted to the special case of the group $\mathsf{SO}(3)$. We finish the paper with some remarks and an outlook.

2. Background

Let G be a locally compact group with left Haar measure μ and identity element e. Consider a finite data set $\mathcal{S} = \{(x_j, \xi_j) \in G \times \mathbb{C} : j = 1, \ldots, M\}$. For notational convenience we write $\mathcal{X} = \{x_1, \ldots, x_M\}$. We are mainly interested in situations where the points x_j are scattered, i.e. we do not assume the x_j's to be located on a grid. The goal is to determine a function s on G which interpolates the data, i.e. $s(x_j) = \xi_j$ for $j = 1, \ldots, M$. We concentrate here on models of s which are given by a linear combination of translates of a suitable basis function ϕ. More precisely, we try to identify s as

$$s(x) = \sum_{k=1}^{M} \alpha_k \phi(x_k^{-1} x), \tag{2}$$

such that $s(x_j) = \xi_j$ for $j = 1, \ldots, M$ is satisfied. In matrix–vector notation the interpolation problem reads as

$$\mathbf{A}_\phi \boldsymbol{\alpha} = \boldsymbol{\xi}, \tag{3}$$

where $\mathbf{A}_\phi = \left(\phi(x_j^{-1} x_i)\right)_{i,j=1}^{M}$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)^{\mathrm{T}}$ and $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_M)^{\mathrm{T}}$. In order to ensure that system (3) is efficiently solvable in a unique and stable way, the function ϕ has to be chosen in a suitable manner. As in the Euclidean case, the so-called positive definite functions turn out to be a good choice.

Let us briefly summarize some basic material on positive definite functions on locally compact groups. We start with the general definition of positive definiteness.

A function $\phi \in C(G)$ is called *positive definite* if

$$\sum_{i=1}^{M} \sum_{j=1}^{M} c_i \overline{c_j} \phi(x_i^{-1} x_j) \geqslant 0 \tag{4}$$

for all $c_1, \ldots, c_M \in \mathbb{C}$, $x_1, \ldots, x_M \in G$ and all $M \in \mathbb{N}$. The function ϕ is called *strictly positive definite* if the left-hand side of (4) is strictly greater than zero for pairwise distinct sampling points $x_j \in G$.

We include continuity of the function in the definition since we are dealing exclusively with continuous positive definite functions.

We denote the set of positive definite functions on G by $P(G)$. The following proposition collects some well-known facts on positive definite functions.

Proposition 2.1. *Let $\phi, \psi \in P(G)$ and $\lambda \in [0, \infty)$. Then we have*

(i) $\phi + \psi,\ \lambda\phi,\ \phi \cdot \psi \in P(G)$,
(ii) $\phi = \widetilde{\phi}$, *where* $\widetilde{\phi}(x) = \overline{\phi(x^{-1})}$,
(iii) $\phi(e) \geqslant 0$ *and* $|\phi(x)| \leqslant \phi(e)$ *for all* $x \in G$.

3. Stability results

In this section we generalize an argument, first used in [15] for scattered data interpolation problems on Euclidean spheres, to state a stability result for interpolation matrices associated with positive definite basis functions on locally compact groups. The ideas of [15] were later adopted by the authors of [11] in order to get stability results for the scattered data interpolation by well-localized trigonometric kernels. We will present an estimate for the eigenvalues and hence for the condition number of the interpolation matrix $\mathbf{A}_\phi$ for well-localized positive definite functions ϕ on locally compact groups.

Clearly the distribution of our sampling points x_j on the group G impacts the condition number of $\mathbf{A}_\phi$. In order to quantify the distribution of the points $\mathcal{X} = \{x_1, \ldots, x_M\}$, we assume the existence of a left translation invariant metric d on G, i.e. a metric d with $d(x, y) = d(zx, zy)$ for all $x, y, z \in G$. This assumption might look like a serious restriction at a first glance, but due to a theorem of Birkhoff and Kakutani there is always a left translation invariant metric on G, provided the topology on G has a countable basis at the identity element e (see [13]).

With respect to the metric d, the *separation distance* q of a given set $\mathcal{X} = \{x_1, \ldots, x_M\}$ is defined by

$$q := \min_{\substack{i,j=1,\ldots,M \\ i \neq j}} d(x_i, x_j). \tag{5}$$

We call a sampling set $\mathcal{X}$ *q-separated* if its separation distance is q.

We follow the lines of [15] and partition our group G in disjoint shells away from the identity element. This is done in the following definition.

Definition 3.1. For $q > 0$ and $m \in \mathbb{N}_0$, let

$$R_{q,m} := \{x \in G : mq \leqslant d(x, e) < (m+1)q\}. \tag{6}$$

For a sampling set $\mathcal{X} = \{x_1, \ldots, x_M\}$ and $l \in \{1, \ldots, M\}$ we denote by

$$\mathcal{X}_l = \{x_l^{-1} x_j \in G : j = 1, \ldots, M\}$$

the corresponding translated sampling set.

Furthermore, we define $R_{\mathcal{X},q,m} := R_{q,m} \cap \mathcal{X}$ and $|R_{\mathcal{X},q,m}| := \mathrm{card}(R_{\mathcal{X},q,m}) \leqslant M < \infty$.

Remark. We obviously have

(i) $e \in \mathcal{X}_l$ for all $l \in \{1, \dots, M\}$,
(ii) $\mathcal{X}$ is q-separated if and only if $\mathcal{X}_l$ is q-separated for all $l \in \{1, \dots, M\}$.

Now we have collected the main ingredients to state our general stability result. The theorem provides estimates for the largest eigenvalue $\lambda_{\max}(\mathbf{A}_\phi)$ and the smallest eigenvalue $\lambda_{\min}(\mathbf{A}_\phi)$ of the interpolation matrix $\mathbf{A}_\phi$, which enables us to bound the condition number

$$\mathsf{cond}(\mathbf{A}_\phi) = \lambda_{\max}(\mathbf{A}_\phi)/\lambda_{\min}(\mathbf{A}_\phi).$$

The bounds only depend on the localization property of the underlying basis function and the separation distance q of the given sampling set.

Theorem 3.2. *Let $\mathcal{X} \subset G$ be q-separated and $k > 0$. If the function $\phi \in P(G)$ satisfies the decay property*

$$|\phi(x)| \leqslant \frac{C}{(d(x,e))^k}$$

for all $x \in G$ with $d(x,e) \geqslant q$, then the following estimates for the smallest and the largest eigenvalue of the interpolation matrix $\mathbf{A}_\phi$ hold true.

(i) $\phi(e) - \frac{C}{q^k} \sum_{m=1}^{\infty} |R_{\mathcal{X}_{l_1},q,m}| m^{-k} \leqslant \lambda_{\min}(\mathbf{A}_\phi) \leqslant \phi(e)$,
(ii) $\phi(e) \leqslant \lambda_{\max}(\mathbf{A}_\phi) \leqslant \phi(e) + \frac{C}{q^k} \sum_{m=1}^{\infty} |R_{\mathcal{X}_{l_2},q,m}| m^{-k}$

for some $l_1, l_2 \in \{1, \dots, M\}$.

Proof. We have $\sum_{i=1}^{M} \lambda_i = \mathsf{tr}(\mathbf{A}_\phi) = M \cdot \phi(e)$, and from this we immediately get

$$\lambda_{\min}(\mathbf{A}_\phi) \leqslant \phi(e) \leqslant \lambda_{\max}(\mathbf{A}_\phi).$$

Now let λ be an arbitrary eigenvalue of $\mathbf{A}_\phi$. Then by Gershgorin's Theorem we get for some $l \in \{1, \dots, M\}$,

$$\begin{aligned} |\lambda - \phi(e)| &\leqslant \sum_{\substack{j=1 \\ j \neq l}}^{M} |\phi(x_l^{-1} x_j)| = \sum_{m=1}^{\infty} \sum_{x_l^{-1} x_j \in R_{q,m}} |\phi(x_l^{-1} x_j)| \\ &\leqslant \sum_{m=1}^{\infty} \sum_{x_l^{-1} x_j \in R_{q,m}} \frac{C}{(d(x_l^{-1} x_j, e))^k} \leqslant C \sum_{m=1}^{\infty} |R_{\mathcal{X}_l,q,m}| \max_{x_l^{-1} x_j \in R_{q,m}} (d(x_l^{-1} x_j, e))^{-k} \\ &= C \sum_{m=1}^{\infty} |R_{\mathcal{X}_l,q,m}| (mq)^{-k}. \end{aligned}$$

From this both estimates follow. □

Obviously these estimates only make sense if the series converges. More precisely, since $\mathbf{A}_\phi$ is positive semidefinite we should require that

$$\frac{C}{q^k} \sum_{m=1}^{\infty} |R_{\mathcal{X}_l,q,m}| m^{-k} \leqslant \phi(e). \tag{7}$$

Before we may be able to put a condition on C such that (7) is satisfied, we certainly need an estimate for the quantity $|R_{\mathcal{X},q,m}|$ for a q-separated sampling set $\mathcal{X}$ in G. The following lemma turns out to be a useful tool to manage this.

Lemma 3.3. *Let $q > 0$ and $m \in \mathbb{N}$. Then for any q-separated set $\mathcal{X} \subset G$ we have*

$$\mu\left(\mathcal{B}_{q/2}(e)\right) \cdot |R_{\mathcal{X},q,m}| \leqslant \mu\left(\mathcal{B}_{(m+3/2)q}(e)\right) - \mu\left(\mathcal{B}_{(m-1/2)q}(e)\right),$$

where $\mathcal{B}_r(x) := \{y \in G : d(x,y) < r\}$ denotes the open ball around x with radius r.

Proof. Using the triangle inequality we easily obtain

(i) $\mathcal{B}_{q/2}(x) \cap \mathcal{B}_{q/2}(y) = \emptyset$ for all $x, y \in \mathcal{X}$,
(ii) $\mathcal{B}_{q/2}(x) \subset \left(\mathcal{B}_{(m+3/2)q}(e) \setminus \mathcal{B}_{(m-1/2)q}(e)\right)$ for all $x \in R_{\mathcal{X},q,m}$.

This implies

$$\bigcup_{y \in R_{\mathcal{X},q,m}} \mathcal{B}_{q/2}(y) \subset \left(\mathcal{B}_{(m+3/2)q}(e) \setminus \mathcal{B}_{(m-1/2)q}(e)\right)$$

and with the equality

$$\begin{aligned}
\mu\Big(\bigcup_{y \in R_{\mathcal{X},q,m}} \mathcal{B}_{q/2}(y)\Big) &= \sum_{y \in R_{\mathcal{X},q,m}} \mu\left(\mathcal{B}_{q/2}(y)\right) = \sum_{y \in R_{\mathcal{X},q,m}} \mu\left(y^{-1}\mathcal{B}_{q/2}(y)\right) \\
&= \sum_{y \in R_{\mathcal{X},q,m}} \mu(\{y^{-1}x : \underbrace{d(x,y)}_{d(y^{-1}x,e)} < \frac{q}{2}\}) = \sum_{y \in R_{\mathcal{X},q,m}} \mu\left(\mathcal{B}_{q/2}(e)\right) \\
&= |R_{\mathcal{X},q,m}| \cdot \mu\left(\mathcal{B}_{q/2}(e)\right)
\end{aligned}$$

we can conclude

$$\begin{aligned}
|R_{\mathcal{X},q,m}| \cdot \mu\left(\mathcal{B}_{q/2}(e)\right) &= \mu\Big(\bigcup_{y \in R_{\mathcal{X},q,m}} \mathcal{B}_{q/2}(y)\Big) \leqslant \mu\left(\mathcal{B}_{(m+3/2)q}(e) \setminus \mathcal{B}_{(m-1/2)q}(e)\right) \\
&= \mu\left(\mathcal{B}_{(m+3/2)q}(e)\right) - \mu\left(\mathcal{B}_{(m-1/2)q}(e)\right). \qquad \square
\end{aligned}$$

In order to make the general results more precise we have to work on concrete groups. Moreover, we have to show how to construct positive definite functions with suitable decay properties. This will be done in the following sections.

4. Construction of positive definite functions

There are several ways of constructing positive definite functions on a group. In this section we concentrate on the relation between representation theory of locally compact groups and positive definite functions. Let us briefly recall the one-to-one relation between continuous unitary representations of the group G and positive definite functions on G.

Let $(\pi, \mathcal{H}_\pi)$ be a unitary representation of G, i.e. π is a homomorphism from G into the group of unitary operators on the Hilbert space $\mathcal{H}_\pi$ which is continuous with respect to the strong operator topology. It is very easy to see that for every $v \in \mathcal{H}_\pi$ the function

$$\phi : G \to \mathbb{C}, \quad \phi(x) = \langle v, \pi(x)v \rangle \tag{8}$$

is continuous and positive definite on G. Conversely, starting with a continuous positive definite function ϕ on G there is always a unitary representation $(\pi, \mathcal{H}_\pi)$ such that (8) holds (see [8]).

The set $P(G)$ is obviously a convex cone. The extremal points of this cone are precisely the irreducible unitary representations of G. Now one might try to construct positive definite functions using the irreducible unitary representations of the group G (see [10]). However, this approach requires the ability to describe these representations explicitly. Unfortunately this is in general a hard problem, especially for non-abelian structures. But if the underlying group is a Lie group we can come up with another unitary representation to construct positive definite functions. Let us now briefly describe this construction. Since in this paper we deal with matrix Lie groups exclusively we restrict ourselves to this case, although the construction works for the general case as well. For more details on Lie groups we refer to the monographs [16,19].

Hence for the remainder of the section let G be a matrix Lie group, i.e. G is a closed subgroup of $\mathsf{GL}(n)$. Recall that the Lie algebra $\mathfrak{g}$ of a matrix Lie group consists of all $n \times n$ matrices such that $\exp(tY) \in G$ for all $t \in \mathbb{R}$. Let $\mathsf{End}(\mathfrak{g})$ denote the algebra of linear operators on $\mathfrak{g}$. The Killing form on $\mathfrak{g}$ is the bilinear form given by

$$\kappa : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}, \quad \kappa(X, Y) = \mathsf{tr}(\mathrm{ad}(X)\mathrm{ad}(Y)),$$

where $\mathrm{ad} : \mathfrak{g} \to \mathsf{End}(\mathfrak{g})$ is defined by $\mathrm{ad}(X)Y = XY - YX$.

There is a natural representation of G on its Lie algebra $\mathfrak{g}$. This representation $\mathrm{Ad} : \mathrm{G} \to \mathsf{GL}(\mathfrak{g})$ is called the adjoint representation of G and is defined as

$$\mathrm{Ad}(y)X := yXy^{-1}.$$

The crucial point here is that for a compact semisimple Lie group the bilinear form

$$\beta(X, Y) := -\kappa(X, Y)$$

gives an inner product on $\mathfrak{g}$, and, moreover, the adjoint representation Ad is a unitary representation on the associated Lie algebra equipped with the inner product β.

Recall that a Lie group G is called semisimple if the Killing form κ is non-degenerate, i.e. if there is no non-zero element $X \in \mathfrak{g}$ with $\kappa(X, Y) = 0$ for all $Y \in \mathfrak{g}$.

According to the above described relation between unitary group representations and functions in $P(G)$ we obtain positive definite functions on a compact semisimple Lie group by

$$\phi(x) = \beta(Y, \mathrm{Ad}(x)Y), \quad Y \in \mathfrak{g}. \tag{9}$$

5. Application to the rotation group

We now focus on the group of rotations in the Euclidean space $\mathbb{R}^3$, i.e.

$$\mathsf{SO}(3) = \{A \in \mathsf{GL}(3, \mathbb{R}) : A^T A = I, \ \det A = 1\}.$$

The rotation group is a compact semisimple Lie group. The Lie algebra of $\mathsf{SO}(3)$ is given by

$$\mathfrak{so}(3) = \{X \in \mathbb{R}^{3\times 3} : X = -X^T\},$$

and the Killing form on $\mathfrak{so}(3)$ simplifies to $\kappa(X, Y) = \mathsf{tr}(X\,Y)$.

According to our considerations above we immediately obtain a family of positive definite functions on $\mathsf{SO}(3)$ by

$$\phi_Y(A) = -\mathsf{tr}(Y\mathrm{Ad}(A)Y) = -\mathsf{tr}(YA\,YA^{-1}), \quad Y \in \mathfrak{so}(3). \tag{10}$$

In order to apply the results of the preceding sections to the rotation group, we certainly need an explicit formula for the Haar measure and also a translation invariant metric on $\mathrm{SO}(3)$. To get an explicit formula for the Haar measure one usually uses the parameterization of $\mathrm{SO}(3)$ in terms of the Euler angles $(\varphi_1, \theta, \varphi_2) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$. This parameterization allows us to write an element $A \in \mathrm{SO}(3)$ as a product of three fundamental matrices (see [9]). More precisely, we have

$$A = A(\varphi_1, \theta, \varphi_2) = S(\varphi_2)R(\theta)S(\varphi_1),$$

where

$$S(t) = \begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos t & -\sin t \\ 0 & \sin t & \cos t \end{pmatrix}.$$

The Haar integral of a function f on $\mathrm{SO}(3)$ now reads as

$$\int_{SO(3)} f(A)\,\mathrm{d}\mu(A) = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} f(\varphi_1, \theta, \varphi_2) \sin\theta \,\mathrm{d}\varphi_1 \,\mathrm{d}\theta \,\mathrm{d}\varphi_2.$$

Besides the parameterization via Euler angles, the identification of $\mathrm{SO}(3)$ with the so-called three-dimensional projective space is of some importance to us. Let K_π be the closed ball of radius π in $\mathbb{R}^3$ and identify antipodal points. This is the three-dimensional projective space (see [9]). An element $A \in \mathrm{SO}(3)$ is identified with a point in the projective space K_π by $A \to \omega x$, where x satisfying $Ax = x$ and $\|x\| = 1$ is the rotation axis and ω is the rotation angle of A which can be chosen in $[0, \pi]$. In this parameterization an element $r = (r_1, r_2, r_3) \in K_\pi$ corresponds to a rotation $A \in \mathrm{SO}(3)$ as follows:

$$A = A(r) = \begin{cases} \begin{pmatrix} \widehat{r_1}^2 C_r + c_r & \widehat{r_1}\widehat{r_2} C_r + \widehat{r_3} s_r & \widehat{r_1}\widehat{r_3} C_r - \widehat{r_2} s_r \\ \widehat{r_1}\widehat{r_2} C_r - \widehat{r_3} s_r & \widehat{r_2}^2 C_r + c_r & \widehat{r_2}\widehat{r_3} C_r + \widehat{r_1} s_r \\ \widehat{r_1}\widehat{r_3} C_r + \widehat{r_2} s_r & \widehat{r_2}\widehat{r_3} C_r - \widehat{r_1} s_r & \widehat{r_3}^2 C_r + c_r \end{pmatrix} & \text{if } r \neq 0, \\ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \text{if } r = 0, \end{cases} \tag{11}$$

where $C_r = (1 - \cos\|r\|_2)$, $c_r = \cos\|r\|_2$, $s_r = \sin\|r\|_2$ and $\widehat{r} = \frac{r}{\|r\|_2}$ for $r \neq 0$.

It is easy to see that

$$d(A, B) := \omega(B^{-1}A)$$

defines a translation invariant metric on $\mathrm{SO}(3)$. We are now ready to apply the results of the previous sections to this concrete situation. At first we will derive an estimate for the quantity $|R_{\mathcal{X},q,m}|$ in case of the rotation group.

Lemma 5.1. *For $q \in (0, \pi]$ let $\mathcal{X} \subset \mathrm{SO}(3)$ be a q-separated set of points. Then we have*

$$|R_{\mathcal{X},q,m}| \leqslant 141 m^2$$

for all $m \in \mathbb{N}$.

Proof. For a class function f on $\mathrm{SO}(3)$ there is a uniquely determined $\tilde{f} : [0, \pi] \to \mathbb{C}$, such that $f(A) = \tilde{f}(\omega(A))$ for all $A \in \mathrm{SO}(3)$. The Haar integral for a class function now reads as (cf. [5, p. 260])

$$\int_{SO(3)} f(A)\,\mathrm{d}\mu(A) = \int_{SO(3)} \tilde{f}(\omega(A))\,\mathrm{d}\mu(A) = \frac{2}{\pi}\int_0^{\pi} \tilde{f}(x)\sin^2\left(\frac{x}{2}\right)\mathrm{d}x. \tag{12}$$

By Lemma 3.3 we know that

$$|R_{\mathcal{X},q,m}| \leqslant \frac{\mu\left(\mathcal{B}_{(m+3/2)q}(I)\right) - \mu\left(\mathcal{B}_{(m-1/2)q}(I)\right)}{\mu\left(\mathcal{B}_{q/2}(I)\right)}. \tag{13}$$

We estimate the numerator from above and the denominator from below separately.

Using (12) we get

$$\begin{aligned}
\mu\left(\mathcal{B}_{(m+3/2)q}(I)\right) - \mu\left(\mathcal{B}_{(m-1/2)q}(I)\right) &= \int_{SO(3)} \left(\mathbb{1}_{(\mathcal{B}_{(m+3/2)q}(I))} - \mathbb{1}_{(\mathcal{B}_{(m-1/2)q}(I))}\right)\mathrm{d}\mu(A)\\
&= \int_{SO(3)} \mathbb{1}_{\{A\in SO(3):(m-1/2)q\leqslant\omega(A)<(m+3/2)q\}}\,\mathrm{d}\mu(A)\\
&= \frac{2}{\pi}\int_{(m-1/2)q}^{(m+3/2)q} \sin^2\left(\frac{x}{2}\right)\mathrm{d}x\\
&\leqslant \frac{2}{\pi}\int_{(m-1/2)q}^{(m+3/2)q} \left(\frac{x}{2}\right)^2\mathrm{d}x\\
&= \frac{q^3}{\pi}\left(m^2 + m + \frac{7}{12}\right).
\end{aligned}$$

On the other hand, using $\sin x \geqslant x - \frac{x^3}{6}$ for all $x \geqslant 0$, we obtain

$$\begin{aligned}
\mu\left(\mathcal{B}_{q/2}(I)\right) &= \int_{SO(3)} \mathbb{1}_{(\mathcal{B}_{q/2}(I))}\,\mathrm{d}\mu(A) = \frac{2}{\pi}\int_0^{q/2}\sin^2\left(\frac{x}{2}\right)\mathrm{d}x\\
&\geqslant \frac{2}{\pi}\int_0^{q/2}\left(\frac{x}{2} - \frac{x^3}{48}\right)^2\mathrm{d}x = \frac{2}{\pi}\left(\frac{q^3}{96} - \frac{q^5}{7680} + \frac{q^7}{2\,064\,384}\right).
\end{aligned}$$

Now consider

$$\gamma(q) := \frac{q^3}{96} - \frac{q^5}{7680} + \frac{q^7}{2\,064\,384} - \frac{q^3}{109}.$$

Then it is easy to check that

$$\gamma(q) \neq 0 \ \ \forall q \in (0, \pi] \quad \text{and} \quad \gamma(1) > 0.$$

This implies

$$\mu\left(\mathcal{B}_{q/2}(I)\right) \geqslant \frac{2}{\pi}\left(\frac{q^3}{96} - \frac{q^5}{7680} + \frac{q^7}{2\,064\,384}\right) \geqslant \frac{2}{\pi}\cdot\frac{q^3}{109}$$

for all $q \in (0, \pi]$. Thus we can finally conclude

$$|R_{\mathcal{X},q,m}| \leqslant \frac{\frac{q^3}{\pi}\left(m^2 + m + \frac{7}{12}\right)}{\frac{2}{\pi} \cdot \frac{q^3}{109}} \leqslant 141 m^2 \tag{14}$$

for all $m \in \mathbb{N}$. $\square$

Remark. Note that

$$\lim_{q \to 0} \frac{\mu\left(\mathcal{B}_{(m+3/2)q}(I)\right) - \mu\left(\mathcal{B}_{(m-1/2)q}(I)\right)}{\mu\left(\mathcal{B}_{q/2}(I)\right)} = 48m^2 + 48m + 28$$

which is therefore the best estimate for arbitrary $q \in (0, \pi]$ we can hope for using the approach of Lemma 3.3. Our first estimate in (14) only differs by a factor less than 1.14 for all $m \in \mathbb{N}$.

Now we are able to state our stability result for scattered data interpolation by positive definite functions on $\mathsf{SO}(3)$. By $\zeta(x)$ we denote the Riemann zeta function evaluated at x.

Theorem 5.2. *For $q \in (0, \pi]$ let $\mathcal{X} \subset \mathsf{SO}(3)$ be a q-separated set. Assume that the positive definite function $\phi : \mathsf{SO}(3) \to \mathbb{C}$ satisfies*

$$|\phi(A)| \leqslant \frac{C}{[\omega(A)]^k}$$

for some $k > 3$ and all $A \in \mathsf{SO}(3)$ with $\omega(A) \geqslant q$. Then we have the following estimate for the eigenvalues of the associated interpolation matrix $\mathbf{A}_\phi$:

$$\phi(I) - \frac{141\zeta(k-2)C}{q^k} \leqslant \lambda_{\min}(\mathbf{A}_\phi) \leqslant \phi(I) \leqslant \lambda_{\max}(\mathbf{A}_\phi) \leqslant \phi(I) + \frac{141\zeta(k-2)C}{q^k}.$$

Proof. This follows directly from Theorem 3.2 with Lemma 5.1. $\square$

In order to use Theorem 5.2 for applicable stability results we should require (cf. (7))

$$\frac{141\zeta(k-2)C}{q^k} < \phi(I). \tag{15}$$

Our next objective is to construct positive definite functions on $\mathsf{SO}(3)$ with good decay properties. In order to do so we apply (10).

Lemma 5.3. *Let $u, v, w \in \mathbb{R}$. Then the function*

$$\begin{aligned}\phi_{u,v,w}(A) = {} & u^2 a_{33} + v^2 a_{22} + w^2 a_{11} - uv(a_{23} + a_{32}) + uw(a_{13} + a_{31}) \\ & - vw(a_{12} + a_{21}),\end{aligned}$$

where $A = (a_{ij})_{i,j=1}^3$, is positive definite and continuous on $\mathsf{SO}(3)$.

Proof. For $u, v, w \in \mathbb{R}$ we have

$$Y := \begin{pmatrix} 0 & u & v \\ -u & 0 & w \\ -v & -w & 0 \end{pmatrix} \in \mathfrak{so}(3).$$

Then (10) with Proposition 2.1 gives the continuous positive definite function

$$\phi_{u,v,w}(A) = \tfrac{1}{2}\phi_Y(A) = -\tfrac{1}{2}\mathsf{tr}(Y A Y A^T).$$

We use $A^T = A^{-1} = \frac{\mathsf{adj}(A)}{\det(A)} = \mathsf{adj}(A)$ to get $a_{ij} = (-1)^{i+j}\det(A_{i,j})$, where $A_{i,j}$ is the matrix that arises when we remove the *i*-th row and *j*-th column from A. Now a direct computation gives us the desired formula. □

In terms of Euler angles the function $\phi_{u,v,w}$ reads as

$$\begin{aligned}\phi_{u,v,w}(\varphi_1, \theta, \varphi_2) = {} & u^2 \cos\theta + v^2(\cos\theta\cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2) \\ & + w^2(\cos\varphi_1\cos\varphi_2 - \cos\theta\sin\varphi_1\sin\varphi_2) \\ & + uv(\sin\theta(\cos\varphi_1 - \cos\varphi_2)) + uw(\sin\theta(\sin\varphi_1 + \sin\varphi_2)) \\ & - 2vw(\sin^2(\theta/2)\sin(\varphi_1 - \varphi_2)).\end{aligned}$$

For the remainder of this section we will construct concrete functions Φ_n out of the family $\phi_{u,v,w}$ and show in detail how an estimate for the condition number of $\mathbf{A}_{\Phi_n}$ can be computed. In order to get well-localized basis functions, we start with a normalized positive definite function Φ_1 that has a unique global maximum at the identity element. Then we can use basic properties about positive definiteness to get basis functions with fast decay.

By Proposition 2.1 and Lemma 5.3 the functions

$$\Phi_n(A) := \frac{1}{4^n}\left(\phi_{0,1,0}(A) + \phi_{0,0,1}(A) + 2\right)^n$$

are positive definite and continuous for all $n \in \mathbb{N}$.

Using Euler angles Φ_n can be written as

$$\Phi_n(\varphi_1, \theta, \varphi_2) = \left(\frac{\cos^2(\theta/2)\cos(\varphi_1 + \varphi_2) + 1}{2}\right)^n.$$

Now it is more convenient to use the representation in the projective space (cf. (11)) to get a result on the localization property of Φ_n. Therefore let the rotation $A \in \mathsf{SO}(3)\backslash\{I\}$ be represented by the vector $r = (r_1, r_2, r_3) \in K_\pi\backslash\{0\}$. Using this parameterization we obtain for all $A \in \mathsf{SO}(3)\backslash\{I\}$

$$\begin{aligned}|\Phi_1(A)| = |\Phi_1(r)| &= \left|\frac{3(r_1^2 + r_2^2) + 2r_3^2 + (r_1^2 + r_2^2 + 2r_3^2)\cos\|r\|_2}{4\|r\|_2^2}\right| \\ &\leqslant \frac{\|r\|_2^2(3 + \cos\|r\|_2) + r_3^2(\cos\|r\|_2 - 1)}{4\|r\|_2^2} \\ &\leqslant \frac{3 + \cos\|r\|_2}{4} = \frac{3 + \cos\omega(A)}{4}.\end{aligned}$$

Remark. Note that if $r_3 = 0$ we get $|\Phi_1(A)| = \frac{3+\cos\omega(A)}{4}$.

We have $\Phi_1(I) = 1$, and so the estimate above, in turn, gives us

$$|\Phi_n(A)| \leqslant \left(\frac{3+\cos\omega(A)}{4}\right)^n \tag{16}$$

for all $A \in \mathrm{SO}(3)$. Inequality (16) shows that Φ_n is a well-localized basis function for sufficiently large n and that now leads to good condition numbers of the associated interpolation matrices.

Theorem 5.4. *Let $q \in (0, \pi]$ and $\mathcal{X} \in \mathrm{SO}(3)$ be a q-separated sampling set. Then for any $\varepsilon \in (0, 1)$, $k > 3$ and $n \in \mathbb{N}$ with $n \geqslant \frac{\log(141\zeta(k-2)) + k(\log\pi - \log q) - \log\varepsilon}{\log 4 - \log(3+\cos q)}$, we get*

$$\mathrm{cond}(\mathbf{A}_{\Phi_n}) \leqslant \frac{1+\varepsilon}{1-\varepsilon}.$$

Proof. We have

$$|\Phi_n(A)| \leqslant \left(\frac{3+\cos\omega(A)}{4}\right)^n \leqslant \left(\frac{3+\cos q}{4}\right)^n \leqslant \frac{q^k\varepsilon}{141\zeta(k-2)\pi^k} \leqslant \frac{q^k\varepsilon}{141\zeta(k-2)[\omega(A)]^k}$$

for all $A \in \mathrm{SO}(3)$ with $\omega(A) \geqslant q$. Hence we may use $C := \frac{q^k\varepsilon}{141\zeta(k-2)}$ in Theorem 5.2 to get

$$\lambda_{\min}(\mathbf{A}_{\Phi_n}) \geqslant 1-\varepsilon \quad \text{and} \quad \lambda_{\max}(\mathbf{A}_{\Phi_n}) \leqslant 1+\varepsilon,$$

respectively. □

In this proof we have used very rough estimates which lead to a strong condition on our parameter n that has to be satisfied to get the result above. With a more detailed analysis of our basis functions Φ_n, we can weaken the condition on n and even get explicit estimates for the eigenvalues of the associated interpolation matrix $\mathbf{A}_{\Phi_n}$ for each n.

Obviously we want to choose our localization constant C as small as possible. On the other hand, we have

$$C \geqslant q^k \cdot \max_{\substack{A \in SO(3) \\ |\omega(A)| = q}} |\Phi_n(A)| = q^k \left(\frac{3+\cos q}{4}\right)^n. \tag{17}$$

The following lemma shows that under some mild conditions we can indeed choose our localization constant C in the optimal way (17).

Lemma 5.5. *Let $q \in (0, \pi]$, $k > 0$. Then for all $n > \max\left\{\frac{6k}{\pi}, \frac{2\pi k}{q^2}, \frac{k(\log\pi - \log q)}{\log(3+\cos q) - \log 2}\right\}$ the following holds true:*

$$x^k \left(\frac{3+\cos x}{4}\right)^n \leqslant q^k \left(\frac{3+\cos q}{4}\right)^n \quad \forall x \in [q, \pi].$$

Proof. We consider the function

$$\varphi(x) = x^k \left(\frac{3+\cos x}{4}\right)^n.$$

The assumption $n > \frac{6k}{\pi}$ implies that φ' has exactly one zero x_0 in $(0, \frac{\pi}{2}]$ and exactly one zero x_1 in $(\frac{\pi}{2}, \pi)$. It is easy to see that φ attains a local maximum in x_0 and a local minimum in

x_1. Furthermore, the assumption $n \geqslant \frac{2\pi k}{q^2}$ ensures that $x_0 \leqslant q$. Since $n \geqslant \frac{k(\log \pi - \log q)}{\log(3+\cos q) - \log 2}$ implies $\varphi(\pi) \leqslant \varphi(q)$ we can conclude $\varphi(x) \leqslant \varphi(q)$ for all $x \in [q, \pi]$. □

We are able to state a more precise stability result for interpolation problems using our basis functions Φ_n.

Theorem 5.6. *Let $q \in (0, \pi]$ and $\mathcal{X} = \{A_i \in \mathsf{SO}(3) : i = 1, \ldots, M\}$ be a q-separated set of sampling points.*

Then for any $k > 3$ and $n \in \mathbb{N}$ with $n > \max\left\{\frac{6k}{\pi}, \frac{2\pi k}{q^2}, \frac{k(\log \pi - \log q)}{\log(3+\cos q) - \log 2}, \frac{\log(141\zeta(k-2))}{\log 4 - \log(3+\cos q)}\right\}$ we get

(i) $0 < 1 - 141\zeta(k-2)\left(\frac{3+\cos q}{4}\right)^n \leqslant \lambda_{\min}(\mathbf{A}_{\Phi_n}) \leqslant 1$,

(ii) $1 \leqslant \lambda_{\max}(\mathbf{A}_{\Phi_n}) \leqslant 1 + 141\zeta(k-2)\left(\frac{3+\cos q}{4}\right)^n$.

Proof. With (16) and Lemma 5.5 we immediately get

$$|\Phi_n(A)| \leqslant \left(\frac{3+\cos\omega(A)}{4}\right)^n \leqslant \frac{q^k\left(\frac{3+\cos q}{4}\right)^n}{[\omega(A)]^k}$$

for all $A \in \mathsf{SO}(3)$ with $\omega(A) \geqslant q$.

Thus the assumptions of Theorem 5.2 are satisfied for $C := q^k\left(\frac{3+\cos q}{4}\right)^n$.

Finally, we have $0 < 1 - 141\zeta(k-2)\left(\frac{3+\cos q}{4}\right)^n$ if and only if

$$n > \frac{\log(141\zeta(k-2))}{\log 4 - \log(3+\cos q)}. \quad \square \tag{18}$$

Remark. In this section we have constructed well-localized positive definite basis functions on $\mathsf{SO}(3)$ in order to get good estimates for the condition number of the associated interpolation matrix. We would like to point out that, as with positive definite functions in Euclidean spaces, a trade-off principle holds true in our setting. Using the well-known power function techniques, one can show that positive definite basis functions on $\mathsf{SO}(3)$ that lead to good stability estimates cause relatively bad estimates for the approximation error (see [18, Corollary 1]).

6. Concluding remarks

Although we applied our stability result in this paper to compact groups exclusively, our general approach as presented in Section 2 is not limited to this case. The proof of the statement given in Theorem 3.2 only depends on the fact that there is a translation invariant metric. As we already mentioned earlier, such a metric always exists in the case of locally compact groups which have a countable basis of neighborhoods at the identity. Among this class one finds all Lie groups. We can generalize our approach furthermore to the case where the underlying set is not necessarily a locally compact group, but a homogeneous space. A homogeneous space is given by a group quotient G/K, where $K \subset G$ is a subgroup. In the case where G is a Lie group and K is a compact subgroup the homogeneous space G/K admits an invariant metric. An invariant or quasi-invariant measure also exists in these cases. Among such examples we find the unit d-sphere in the Euclidean space $\mathbb{R}^{d+1}$ which can be realized as $\mathsf{SO}(d+1)/\mathsf{SO}(d)$. There are a lot more examples which are of quite some relevance in physics. Whereas the d-sphere has been studied in detail by several authors (see for example [15]), other examples have not been considered similarly with regard to scattered data approximation. We plan to study some examples in a forthcoming paper.

Although the general result can be transferred to other settings, the construction of positive definite functions with good decay properties is a problem of its own. In this respect it would be important to have conditions on the representation $(\pi, \mathcal{H}_\pi)$ of the group, which would ensure decay of some order of the positive definite function $\phi(x) = \langle v, \pi(x)v\rangle$. We are not aware of such conditions. On a homogeneous space a positive definite function ϕ is necessarily zonal, i.e. it is constant on double cosets $xKy = \{xky : k \in K\}$. Suitable functions can then be constructed by using convolution structures (see [6,7]).

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